Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201010

FWP and/or subtask Title under FWP: Studies of Nanoscale Structure and Structural Defects in Advanced Materials

FWP Number: MA-015-MACA

Program Scope:
The goal of this program is to study property sensitive nanoscale structure and defects in technologically-important materials such as superconductors, magnets, and other functional materials. Advanced quantitative electron microscopy techniques, such as coherent diffraction, atomic imaging, column-by-column spectroscopy, and phase retrieval methods including electron holography are developed and employed to study material behaviors. Computer simulations and theoretical modeling are carried out to aid the interpretation of experimental data. Fabrication of thin films with tailored microstructure and nano-assemblies to understand materials' electronic and magnetic behaviors is also incorporated.

Major Program Achievements (FY2006):
(1) Fabrication of Permalloy tear-drop-shaped elements to study the effects of edge roughness on magnetic nucleation and switching behavior with comparisons between experiment and micromagnetics simulation; (2) Development of the theoretical framework for magnetostatic shape anisotropy and demagnetization effects to plot the magnetic phase diagram for nanorings with different geometries; (3) Study of $YBa_2Cu_3O_7$ twin boundary structural modification as a function of oxygen ordering and concentration and statistic measurement of local orthorhombicity and oxygen ordering of twining domains using the geometrical phase analysis method; (4) Combined study of the electronic structure of $CaCu_3Ti_4O_{12}$ single crystal using coherent electron diffraction (PARODI method), synchrotron x-ray diffraction, EXAFS and DFT calculations to understand the material's gigantic dielectric behavior; (5) Understanding electron doping and straining effects and the two-band superconductivity in MgB_2 using high-resolution EELS and DFT; (6) Study of corrected behavior of spins and electrons in digitally synthesized $LaMnO_3/SrMnO_3$ multilayer films to understand interfacial charge transfer and ferromagnetic to antiferromagnetic transition; (7) Study of crystal structure of $Ca_3Co_4O_9$ thermoelectric material with incommensurate modulation; (8) Instrumentation development on phase plate for optimization of imaging single molecules with aberration corrected microscopes and on fast electron detectors.

Program Impact: The impact of this work is the development of advanced imaging techniques that can be broadly applied to quantitatively characterize a variety of materials and their behavior. Applications to magnetic materials and strongly correlated electron systems including high Tc superconductors are demonstrated.

Interactions: Internal—Superconducting and magnetic materials group, Neutron scattering group, Synchrotron x-ray diffraction group, Solid-state theory group; Center for data intensive computing, and Biology STEM group. External—Columbia University; Stony Brook University; Carnegie Mellon University; Yale University; Argonne National Lab; University of Illinois at Urbana-Champaign; University of Alberta, Canada; University of Oslo, Norway; and University of Bologna, Italy.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
Y. Zhu – APS fellow (2006); Distinguished Science and Technology Award, BNL (2003); Program Committees and symposium co-organizer, MMM (2006), IMC16 (2006), MSA (2006), MRS (2005); Editorial Board of *MICRON*, Adjunct Professor at Dept. of Applied Physics and Mathematics, Columbia University; Dept. of Physics, and Dept. of Materials Science, Stony Brook University; R. Klie – BNL Goldhabor Fellow (2002-2005), J. Lau et al, Best poster Award, 49th Mag, Mag. Mat. conference (2004). J. Lau, National Research Council Postdoc Fellow (2005). 35 invited talks in the last three years at major conferences excluding institution seminars.

Personnel Commitments for FY2006 to Nearest +/- 10%: Y.Zhu (75%), L.Wu (100%), V.Volkov (100%), M.Schofield (90%), M.Beleggia (90%), R.Klie (100%), and J. Zheng (100%).

Authorized Budget (BA):
FY04 BA - $1,598K **FY05 BA -** $1,898K **FY06 BA -** $1,898K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201030

FWP and possible subtask under FWP: Superconducting Materials
FWP Number: MA-012-MABA
Program Scope: This program studies the basic relationships between nanoscale structures and macroscopic properties of superconductors, providing the understanding of the fundamental physics and materials science required for their practical utilization. High temperature superconducting (HTS) cuprates, alloyed MgB_2, and superconductor/magnet heterostructures are systems receiving emphasis.
Major Program Achievements (over duration of support):
1) Enhanced flux pinning in HTS $YBa_2Cu_3O_{7-\delta}$ (YBCO) films by nanometer-scale substrate surface roughness was demonstrated, which resulted in ~ 30% increase in critical current density J_c.

2) Effects of a magnetic substrate on the ac losses of superconducting films were investigated by measuring the losses of an YBCO layer on a magnetic Ni–5 at. % W substrate in perpendicular ac magnetic fields, and using magneto-optical imaging (MOI) technique. At low fields, the losses depended on ac magnetic field amplitude B and film thickness t as $\sim B^3/t$ instead of $\sim B^4/t^3$ for a superconducting film on a nonmagnetic substrate.

3) Nearly complete suppression of flux density peaks at the edge of a superconducting film was observed for the first time by direct MOI imaging the magnetic induction profiles of an YBCO film on a magnetic substrate in perpendicular magnetic fields. This is in a striking contrast to the case of superconducting films on a non-magnetic substrate that display sharp flux density peaks at the edges of the films due to the demagnetization effect.

4) Strong *isotropic* flux pinning was observed for the first time in strong anisotropic HTS at liquid nitrogen temperatures. The very weak angular dependence of J_c around c-axis indicates that the pinning centers in record high-J_c YBCO thick films made on the magnetic substrates are *isotropic* and are not correlated to a particular direction or alignment.

5) Studies of structure, heat capacity, and transmission electron microscopy with electron energy loss spectroscopy were coordinated to probe the changes in superconductivity in MgB_2 when the Mg atoms are progressively replaced by Al. We obtained the first direct evidence for the filling of the hole states in the planar σ band, which are crucial for the high critical temperature in pure MgB_2, by the extra electrons donated by Al. Yet, other property measurements indicated that superconductivity was not destroyed when there was sufficient Al to fill all of the hole states, but it persisted to much higher levels of Al doping. Using a two-band model of superconductivity, fits to the heat capacity data indicated that it is the π band that survives in the heavily doped regime, which is an inversion of the hierarchy of the bands in pure MgB_2.
Program Impact:
Results (1)-(3) suggest that nanoscale substrate surface roughness, magnetic coupling in superconductor/magnet heterostructures can be used to enhance the HTS performance. Results (4) suggest that it is possible to achieve very high J_c without using the additives to YBCO films, and this makes the process and application of HTS easier. Results (5) explain why the critical temperature in MgB_2 falls with dopant concentration.
Interactions:
Cond. Mat. Phys. and Mat. Sci. Dept., CFN, NSLS of BNL, Penn State Univ. (X. X. Xi), Los Alamos Lab (L. Civale, B. Maierov), UC San Diego (I. Schuller), Univ. of Gottengen (C. Jooss), Univ. de Sherbrooke (L. Taillefer), SUNY at Stony Brook (A. Goldstone, S. Sampath and R. Gambino), Amer. Supercon. Inc. (M. Rupich), Specialty Materials Inc. (J. Marzik and A. Kumnik), Florida State (D. Larbalestier), Superconducting Technologies Inc. (B. Moeckly), HyperTech Inc. (M. Tomsic)
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Adjunct Professor of Physics (Li) of State University of New York at Stony Brook, Z. Ye – SUNY President Award for Outstanding Ph. D Graduates (2005), 6 invited talks in FY06.
Personnel Commitments for FY2006 to Nearest +/-10%:
Q. Li (PI) 100%, L. Cooley (Co-PI) 35%, A. Moodenbaugh 40%, H. Wiesmann 5%
Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA - $974K **FY05 BA** - $729K **FY06 BA** - $714K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201050

FWP: Molecular beam epitaxy and nano-structuring of perovskite oxide materials toward an understanding of strongly correlated systems. **FWP Number:** MA-509-MACA
Subtask under FWP: Bulk Materials Synthesis and Characterization.

Program Scope:
Molecular beam epitaxy: We have developed a unique molecular beam epitaxy synthesis technique to synthesize atomically perfect thin films, multilayers, and superlattices containing cuprate high-temperature superconductors (HTS) and other complex oxides. This in turn enables fabrication of HTS heterostructures nanowires and nanodots of unprecedented quality.
Bulk Materials Synthesis: Design, synthesis and characterization of new materials; discovery of new phenomena associated with correlated electron behavior and problems in superconductivity and magnetism.

Major Program Achievements (over duration of support):
Molecular beam epitaxy: The new MBE laboratory, including a clean room with nano-lithography capability, has been set up from scratch. We have developed the technology to synthesize atomically smooth HTS films with 100 %, thus greatly surpassing what used to be the state-of-the-art. We have built custom setups for measurement of resistivity, susceptibility, photo-conductivity, and photo-inducted absorption and a unique system for parallel (32-channel) measurements of R(T) and the Hall effect.
Bulk Materials Synthesis: Discovered colossal magnetoresistance (CMR) effect in Co-doped $FeSb_2$. Synthesized high purity samples of heavy fermion superconductors and discovered unconventional multi-band superconductivity. Synthesized single crystals of Nb_2Se_3, a quasi–1D superconductor with Nb metal chains.

Program impact:
These unique samples enable challenging experiments that deepen our understanding of materials that are governed by correlated electrons, thus providing the scientific base for their optimization and usage. Of particular note is the discovery of a giant proximity effect in the high temperature superconductors, which is stimulating much research worldwide.

Interactions:
Internal: TEM (Zhu), XRD (Hill), nanowires (Misewich), ARPES (Valla, Johnson), NSLS (Kao, Nelson), neutron scattering (Zaliznyak, Gardner), nanotubes (Wang), nanowires arrays (Li).
External: NHMFL (Boebinger), UIUC (Abbamonte), Caltech (Zewail), PSI Zurich (Morenzoni), Berkeley (Dynes), Akron (Djordjevic), Wisconsin (Lagally), Columbia (Osgood), Princeton (Ong), Johns Hopkins (Broholm), Brown (Mitrovic), Notre Dame (Eskildsen), ORNL (Hermann), Sherbrooke (Taillefer), Toronto (Wei), ETH (Degiorgi), San Diego (Maple), Ames (Canfield), Northwestern (Ketterson), Yonsei University Korea (Lee), CEA Grenoble (Lapertot, Flouquet), Brock (Reedyk), Liège (Grandjean).

Recognitions, Honors and Awards (partly attributable to support under this FWP:
Laureate, SPIE Technology Achievement Award
Chair, Conference on Strongly Correlated Electron Materials, San Diego, CA
Chair, Materials Panel, DOE BES Workshop on Research Needs for Superconductivity, Arlington, VA
Member, International Advisory Committee, Institute for Complex Matter, Lausanne, Switzerland.
Member, Editorial Board, *The International Journal of Superconductivity*.
2006, Guest Editor, J. Superconductivity, special issue honoring V. L. Ginzburg.
Member, International Advisory Board, for 13 conferences in 2004-6
44 invited talks at conferences in 2004-6; 25 invited colloquia and seminar talks.

Personnel Commitments for FY2006 to Nearest +/- 10%:
I. Bozovic (40%), G. Logvenov (10%), V. Butko (25%), A. Gozar (0%), A. Bollinger (3%),
C. Petrovic 100%, R. Hu (student) 75%, R. Huang (student) 100%.

Authorized Budget (BA): FY04 BA $ 120K. **FY05 BA** $ 1,615K **FY06 BA** $1,737K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201050

FWP and possible subtask under FWP:
Synthesis and Characterization of Individual Carbon and Perovskite Oxide Nanotubes

FWP Number:
MA-507-MAAA

Program Scope:
Synthesis of carbon and perovskite oxide nanomaterials, individual nanomaterial characterization, and modeling are combined to provide insights toward correlating nanomaterial structure with function.

Major Program Achievements (over duration of support):
- Advances in the synthesis of novel nanomaterials including the development of solid-state synthesis techniques for high-quality oxide nanomaterials. Examples include single-crystalline $Bi_2Fe_4O_9$ cubes and single-crystalline $Ca_{1-x}Sr_xTiO_3$ ($0 \leq x \leq 1$) perovskite nanoparticles with shape changing from cubes to quasi-spheres with decreasing 'x' values. Other oxide synthesis advances include the demonstration of a size- and shape-dependent morphological transformation during the hydrothermal soft chemical transformation of titanate nanostructures into their anatase titania counterparts.
- Developed near edge X-ray absorption fine structure (NEXAFS) spectroscopy as an analytical tool for analysis of order, alignment, phase, defects and crystallinity of nanomaterial samples.
- Synthesis of three-dimensional, dendritic micron-scale spheres composed of alkali metal hydrogen titanate 1D nanostructures (i.e.: nanowires and nanotubes) via a modified hydrothermal technique. Sea-urchin-like assemblies of these 1D nanostructures have been transformed into their hydrogen titanate analogues as well as into their corresponding anatase TiO_2 nanostructured counterparts through a moderate high-temperature annealing dehydration process without destroying the 3D hierarchical structure.
- Developed sensitive spectroscopic tools to determine the electroluminescence emission spectra from individual carbon nanotubes in-situ at a probe station where simultaneous transport studies are performed. Developed techniques for structural determination of the nanotube under probe.
- Functionalization of carbon nanotubes, including weak chemistry functionalization with proteins to explore organic/inorganic hybrid nanomaterials.

Program impact
- TiO_2 nanoparticulate products we have isolated are single-crystalline, of the anatase phase, and of high purity, without impurities arising from brookite or rutile, all of which are desirable characteristics for nanoparticles with potential applications in photocatalysis and other chemical processes.
- We have shown that NEXAFS spectroscopy can be used to determine the surface orientation and the extent of order in vertically aligned carbon nanotube arrays grown on a substrate which provided for a complementary, more nuanced determination of local surface order as compared with SEM analyses.
- We have demonstrated that micron scale assemblies of TiO_2 1D nanostructures are active photocatalysts for the degradation of synthetic Procion Red dye under UV light illumination.
- Discovered new method of optical emission from a single carbon nanotube. Spectroscopic studies of individual carbon nanotubes showed that the electroluminescence spectra depend on the length and diameter of the carbon nanotube. First simultaneous spectroscopy and direct structural determination on same nanotube, showed chiral dependence of metallic tube energy splitting.
- Demonstration of a high sensitivity, highly specific sensor utilizing a protein-functionalized single carbon nanotube FET.

Interactions:
National Synchrotron Light Source, State University of New York at Stony Brook, Argonne National Laboratory, Columbia University, IBM Yorktown Heights, NIST, University of Pennsylvania, Princeton University.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
S.S. Wong – Alfred P. Sloan Foundation Fellowship - 2006.

No. of Invited Talks (National and International Meetings): 8 in FY06

Personnel Commitments for FY2006 to Nearest +/- 10%:
S.S. Wong (50%); J. Misewich (0 %)

Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA $440K **FY05 BA $422K** **FY06 BA $414K**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202010

FWP and possible subtask under FWP
Condensed Matter Physics--X-ray Scattering

FWP Number: PO- 011

Program Scope:
The X-ray Scattering Group carries out basic studies of the structural, electronic and magnetic properties of condensed matter systems using synchrotron x-ray scattering. The Group also develops instrumentation and maintains and operates beamlines at the National Synchrotron Light Source, and at the Advanced Photon Source (APS). Particular emphasis is placed on investigation of surface and interfacial phenomena, including thin films, on electronic and magnetic structure and phase behavior, and on electronic excitations in solids. Current research is focused on strongly correlated electron systems and liquid interfaces and thin films.

Major Program Achievements (over duration of support):
The program has played a significant role in developing and applying resonant x-ray scattering techniques to the study of condensed matter systems, including especially the study of magnetic phenomena and of electronic ordering and excitations in strongly correlated systems. Efforts in the field of liquid interfaces have led to significant discoveries such as surface freezing and surface-induced layering in liquid metals. The X22 beam lines have been among the premier x-ray scattering lines at the NSLS. The group played a leading role in the construction, and operation, of the Complex Materials Consortium-Collaborative Access Team (CMC-CAT) at the APS and the construction of a new sector dedicated to inelastic x-ray scattering (IXS-CDT), which began commissioning in FY06.

Program impact:
The Group's longstanding programs concerned with x-ray resonant phenomena, and with liquid and soft interfaces have been seminal in stimulating related efforts worldwide, and remain among the leading programs in these areas today. Efforts in soft condensed matter led to the creation of a new FWP aimed at understanding nanoscale confinement and the role of self-assembly in soft materials. Work in inelastic x-ray scattering led, with others, to the creation of the IXS-CDT at the APS. Highlights in FY06 include the observation of two magnon scattering in cuprates with inelastic x-ray scattering, the first observation of an orbital 'truncation rod' associated with surface orbital order and the first measurements of the structure of a buried organic thin layer film under applied potential.

Interactions:
The Group typically collaborates with ~20 PIs per year, together with an approximately equal number of students and post docs. This includes significant internal BNL collaboration, both within Condensed Matter Physics and Materials Science and more widely (in particular, the NSLS, CFN, Chemistry) together with external collaborations with universities, other national laboratories and foreign institutions.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
12 invited talks in FY06
Previously:
2 Goldhaber Fellows, 1 Wohlfarth Award, 1 Significant Achievement in Solid State Physics, 1 Presidential Early Career Award, 3 Fellows of the APS, 1 Fellow of AAAS, 1 Brookhaven Engineering Award, 1 Brookhaven Science and Technology Award, Editorial Board Member, J. Phys. Condens. Matter.

Personnel Commitments for FY2006 to Nearest +/- 10%:
John Hill (Group Leader) (70%), Ben Ocko (100%), Mary Upton (50%), Jessica Thomas (50%), Julian Baumert (0%), Scott Coburn (80%, Engineer), Bill Schoenig (100%, technician), Members of the Soft Matter Group (Fukuto and Checco) are also members of the x-ray scattering group, but received no salary support from this FWP.

Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA $1,140,000 **FY05 BA** $1,525,000 **FY06 BA** $1,496,000

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC020201

FWP and possible subtask under FWP:
Neutron Scattering

FWP Number: PO-010

Program Scope: Elastic and inelastic neutron scattering are used to investigate phenomena such as high-temperature superconductivity, charge and spin ordering in doped Mott insulators, low-dimensional and quantum-disordered antiferromagnism, and ferroelectricity. Experiments utilize national and international neutron facilities, especially instrumentation developed and supported by BNL, and single-crystal samples grown at BNL.

Major Program Achievements (over duration of support):
High-Temperature Superconductivity: Discovery and characterization of magnetic order and fluctuations in cuprates; discovery of stripe order in certain cuprates; discovery of universal magnetic spectrum for cuprates.
Doped Mott insulators: Discovery of stripe order in $La_{2-x}Sr_xNiO_{4+\delta}$ and measurement of associated spin waves; checkerboard charge plus magnetic order in $La_{0.5}Sr_{1.5}MnO_4$, $La_{1.5}Sr_{0.5}CoO_4$.
Ferroelectrics: Identification of new structural phase in $Pb(Zr_{1-x}Ti_x)O_3$; characterization of overdamped optical modes and atomic displacement pattern corresponding to polarized nano-domains in relaxor ferroelectrics.
Quantum magnetism: Characterization of dimensional crossover in systems of coupled quantum-spin chains; first observation of magnetic-field-induced order in a quantum-disordered system.
Crystal growth: Growth of very large crystals of $La_{2-x}Ba_xCuO_4$ and $Bi_2Sr_2CaCuO_{8+\delta}$ enabling detailed studies of magnetic excitations in superconductors.
Instrument development: Concept for HYSPEC at the SNS; US-Japan cold triple-axis spectrometer at HFIR

Program impact:
Results on charge-stripe correlations in cuprates have stimulated new theories of the mechanism for high-temperature superconductivity. Identification of structure and polarization direction in optimized piezoelectric $Pb(Zr_{1-x}Ti_x)O_3$ (PZT) has led to predictions of improved performance in atomically-tailored materials.

Interactions:
Internal---Condensed-Matter Physics and Materials Science Dept.: X-ray Scattering Group, Materials Synthesis and Characterization Group, Electron Spectroscopy Group, Theory Group, Superconductivity Group; Center for Functional Nanomaterials: Electron Microscopy Group
External---University of Delaware; Johns Hopkins University; Rutgers University; Virginia Tech; Oak Ridge National Laboratory; National Institute of Standards and Technology; Institute for Solid State Physics, University of Tokyo, Japan; Institute for Materials Research, Tohoku University, Japan; Japanese Atomic Energy Agency; Oxford University, UK; Rutherford-Appleton Laboratory, UK; Laboratoire Léon Brillouin, France; CEA/Grenoble, France; Hahn-Meitner Institute, Berlin, Germany; Forschungszentrum Karlsruhe, Germany; IFW Dresden, Germany

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2 Fellows of the American Physical Society; 1 Fellow of the Neutron Scattering Society of America.
1 Fellow AAAS.
13 invited talks at national and international conferences in FY06.
I. Zaliznyak and S.M. Shapiro---Principle investigators of HYSPEC instrument development team
J.M. Tranquada---Sustained Research Prize, Neutron Scattering Society of America, 2006; Divisional Associate Editor, Physical Review Letters, 2001-present; member, Lehman Review Committee for the Spallation Neutron Source; Program Advisory Committee, NIST Center for Neutron Research.

Personnel Commitments for FY2007 to Nearest +/- 10%:
J. M. Tranquada (group leader) (100%), G. Gu (100%), M. Hücker (100%), L. Passell (consultant, 25%), B. Winn (stationed at ORNL, 100%), G. Xu (100%), I. Zaliznyak (100%), K. Mohanty (100%)

Authorized Budget (BA) for FY04, FY05, FY06: (including Neutron Instrument Development and User Support)
FY04 BA $1591K (+$630K) **FY05 BA** $1836K+$550K **FY06 BA** $1650K+$400K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202020

FWP and possible subtask under FWP:
Condensed Matter Physics—Electron Spectroscopy

FWP Number: PO-016

Program Scope:
The Electron Spectroscopy Group's primary focus is on the electronic structure and dynamics of condensed matter systems. The group carries out studies on a range of materials including strongly correlated systems. A special emphasis is placed on studies of High Tc superconductors and related materials. The primary techniques used include High-Resolution Photoemission and Infra-Red Spectroscopy or Optical Conductivity. The experiments are carried out both within the laboratories in the Condensed Matter Physics and Materials Science Department and at the National Synchrotron Light Source. The emphasis is on the study of the low energy excitations and the nature of the interactions of the latter with their environment. The group has also established a successful pulsed laser deposition facility for the study of thin films. Future plans involve studies of nanoscale systems and will involve close collaboration and work within the newly created Center for Functional Nanomaterials. The group is also heavily involved in the development of new spectroscopy capabilities.

Major Program Achievements (over duration of support):
The program has established one of the leading spectroscopy groups in the world working in the area of strongly-correlated electrons. The group has recently been involved in detailed studies of $La_{2-x}Ba_xCuO_4$ and reported important new insights into the physics of the pseudogap phase, and demonstrated a scaling law relating the superfluid density to the product of the normal state conductivity and the superconducting transition temperature for the high Tc superconducting cuprates. The group was also the first to identify the kink or mass renormalization observed in the nodal direction of the high Tc materials. Further the group has introduced the method of analysis in photoemission involving Momentum Distribution Curves (MDC).

Program Impact:
Using the techniques of photoelectron spectroscopy and optical conductivity, the group has had a major impact in the areas of high Tc superconductivity, magnetic thin films and multilayers and surfaces. This is evidenced by the large number of citations and by the number of invited talks at major international and national conferences.

Interactions:
The Group collaborated with approximately sixty faculty, together with associated students and post docs. This includes significant internal BNL collaboration, both within Condensed Matter Physics and Materials Science Dept. and more widely (in particular, the NSLS, and CFN) together with external collaborations with universities, other national laboratories and foreign institutions.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Previously
2 Fellows of the APS
1 Fellow of the Institute of Physics, U.K.
2001 Brookhaven Science and technology Award

No. of Invited Talks: 12 in FY06

Personnel Commitments for FY2006 to Nearest +/-10%:
Peter D. Johnson (Group Leader, 90%)
Christopher Homes (95%)
Tonica Valla (100%)
Weidong Si (100%)
Hongbo Yang (75%-Research Associate)
F. Loeb (85%)
Jon Rameau (100% - Student)

Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA - $1,525K **FY05 BA - $1,660K** **FY06 BA - $1,660K**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202020

FWP and/or subtask Title under FWP: Magnetostructural Phase Transitions at the Nanoscale

FWP Number: MA-410-MABA

Program Scope:
It is the objective of this research program to investigate magnetostructural phase transformations as the microstructural scale is decreased from bulk to nanoscale in simple model systems. Inherent to this research is characterization of structural and magnetic information including transition temperature effects, lattice distortions, spin polarization and ultrafast dynamics; all are linked by multiscale modeling efforts. Emphasis is placed on how critical exponents/order parameters characterizing the transition evolve with scale and geometry; consequences of strain (system confinement or clamping) and its compensating effects on such transitions are also examined.

Major Program Achievements (over duration of support):
Computational analysis of the influence of intergrain dipolar coupling in exchange-coupled-composite materials has revealed that dipolar and exchange coupling contribute equally in driving the magnetic response of such systems.

Isolated ferromagnetic MnBi nanorods are found to exhibit a first-order magnetostructural over 100 degrees lower than the bulk counterpart; high-temperature x-ray diffraction indicates that the nanophase transformation is fundamentally different from the bulk and is tentatively attributed to dilational strain from the matrix phase.

First-principles calculations of MnBi energy and magnetic moment conclude that the zinc-blende structure is mechanically unstable; setting the in-plane lattice constant of ZnS-type MnBi to equal that of typical semiconductors (such as GaAs) and minimizing E as a function of c/a causes MnBi to become a half-metallic ferromagnet.

Quantitative results from TEM off-axis electron holography obtained on 60-nm-thick Ni films in the vicinity of the ferromagnetic Curie temperature reveal a temperature dependence of the magnetization that implies the existence of multiple magnetic phases of nanometer dimensions.

BNL researchers have recently developed element-specific ferromagnetic resonance (ER-FMR), which enables the study of the dynamics of individual elemental magnetic moments on complex alloy or multilayer structures.

Program impact:
Demonstrated that magnetostructural transitions, and associated extreme responses, may be manipulated in strain-temperature-field parameter space as well as by structuring the materials system on the nanoscale.

Interactions: Columbia University (magnetization dynamics), SUNY Stony Brook (nanostructured magnetocaloric & high-frequency materials); IEN Torino, Italy (magnetostructural response). U. Bologna, Italy (critical exponents); U. Göttingen, Germany (reversal mechanisms); NIST-Gathersberg (nanostructured arrays); NINT-Canada (nanopatterning); National Tsing Hua University, Hsinchu, Taiwan (computational models)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP): (FY06)
(L. H. Lewis): Exhibits Chair, Joint MMM/Intermag Meeting (2007); U. S. Patent award 7,076,959: "Simple Magnetic Field Amplification for Functional Magnetic Materials".
No. of Invited Talks in FY06: 2

Personnel Commitments for FY2006 to Nearest +/- 10%:
L. H. Lewis (75%), D. Arena (10%), M. Schofield (10%); M. Beleggia (10%), Y. Ding (10%)

Authorized Budget (BA) for FY04, FY05, FY06

FY04 BA $410 K **FY05 BA** $300 K **FY06 BA** $450 K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202020

FWP and possible subtask under FWP: Atomistic Transport Mechanisms in Revisible Complex Metal Hydrides
FWP Number: BO-130
Program Scope:
This research program has two major objectives: i) the development of a comprehensive, quantitative understanding of the fundamental, atomic-scale mechanisms underlying the facile reversible hydrogen storage in titanium-doped sodium alanate ($NaAlH_4$), the only complex hydride allowing reversible hydrogen storage known to date; and ii) the utilization of this basic knowledge for the rational screening for novel complex hydride storage materials with properties superior to those of $NaAlH_4$. In contrast to previous research on bulk compounds with complex reaction pathways and microstructures, the present program is based on the use of well-defined model systems and a suite of state-of-the-art surface experiments to achieve a quantitative understanding of the important reaction mechanisms. This approach generates data on systems accessible to first-principles calculations, and allows an unprecedented level of interaction between experiment and theory. Key questions to be addressed include: i) the mechanism of hydrogen dissociation on Al surface doped with Ti; ii) the identification of the predominant carrier of mass transport, and measurements of its diffusion kinetics; and iii) the microscopic reaction mechanisms and their rate-limiting step as NaH and Al react to Na_3AlH_6 and $NaAlH_4$ in the presence of hydrogen.

Major Program Achievements (over duration of support):

As a key step toward identifying H_2 dissociation mechanisms on Ti-doped Al surfaces, STM experiments mapping the Ti distribution in dilute Ti-Al(111) near-surface alloys have concluded with two major findings: i) Ti is kinetically stabilized in surface and near-surface sites as a disordered Ti-Al alloy, whereas theory predicts that Ti should occupy sub-surface sites in equilibrium. And ii) nearest neighbor pairs of Ti atoms are avoided, which produces a large population of second-nearest neighbor Ti-Ti pairs. Under non-equilibrium conditions, as found in hydrogen storage reactions, Ti will thus indeed be available in surface sites to catalyze H_2 dissociation. Surface Ti-atom pairs occur predominantly in a geometry (Ti-Ti spacing and symmetry) predicted to be highly active in H_2 dissociation by our previous density-functional theory calculations.
IR spectroscopy on the interaction of atomic-H with Al(111) model surfaces, combined with theory, provided important insight into the role of surface alanes (AlH_3, Al_2H_6, etc.) in hydrogenation reactions. Our results suggest a surface bonding of small alanes consistent with a high diffusion mobility of these species. Moreover, a clear tendency of alanes to agglomerate is observed at increasing temperature or H-coverage, in sharp contrast with the theoretically predicted fractioning of larger alanes in the limit of zero coverage.
Our work on bulk hydrogen storage materials, finally, has provided evidence of predominant near-surface Ti, and confirmed a major role of alanes (AlH_3) as a primary diffusing species in storage reactions. EXAFS on dehydrogenated Ti-doped sodium alanate showed the transition metal entirely near the surface of metallic Al with a disordered distribution of Ti-Al distances. Hydrogenation experiments, demonstrating that AlH_3 reacts spontaneously with NaH to form $NaAlH_4$ without a catalyst or hydrogen overpressure, suggested the initial formation of mobile alane as a rate-limiting reaction step.

Program impact:

The impact of this project will be to provide a fundamental understanding of the atomic processes leading to the reversible storage of H_2 in complex metal hydrides. This understanding will provide the basis for the development of new higher performance H_2 storage materials.

Interactions:
Yves Chabal, Rutgers University, BNL-CFN, BNL Chemistry and BNL Materials Science & Condensed Matter Physics
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Ewald Wicke Award, 2006, presented at the International Metal Hydride Symposium to Jason Graetz.
Personnel Commitments for FY2006 to Nearest +/- 10%:
P. Sutter (20%), Muckerman (13%), J. Flege (80%), S. Chaudhuri (90%), P. Zahl (100%), Y. Chabal (Contract)

Authorized Budget (BA): FY04, FY05, FY06:
FY04 BA - $N/A **FY05 BA** - $700K **FY06 BA** - $700K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202030

FWP and possible subtask under FWP:
Electronic Properties of Transition-Metal-Compound Nanotubes

FWP Number: PM-002

Program Scope:
Theoretical exploration of interesting electronic properties of transitional metal compound nanotubes, via interplay between the charge, spin, orbital, and lattice degrees of freedom:

- Electronic structure and physical properties of transitional metal compound nanotubes
- Broken symmetries in correlated nanotubes with "frustrated" spin channel
- Lattice properties and potential self-assembly
- Charge and magnetic excitations; propagation of local excitons
- Development of numerical canonical transformation and renormalization for rigorous derivation of low-energy effective Hamiltonian

Major Program Achievements (over duration of support):

- Construction of a systematic technique of quantitatively mapping out the relevant interactions in strongly correlated system, based on first-principles Wannier functions
- Explanation of gapless CDW in bulk TaSe2
- Development of real space method for the study of local excitons
- Explanation of strong anisotropy in NiO and CoO
- Development of finite-temperature time-dependent reduced density functional theory
- Preparation for numerical tools for large-scale computation of nanotubes

Program impact:
Provided insights into behavior of strongly correlated TMO and TMD

Interactions:
Internal:
Electron Spectroscopy, X-ray Scattering, Neutron Scattering, Powder Diffraction, CFN, CSC
External:
Harvard University (Prof. E. Demler), Boston College (Prof. H. Ding) , University of Utah (Prof. D. Mattis), University of Tennessee (A.G. Eguiluz), ORNL (B.C. Larson, P. Kent) , Tamkang University, Taiwan (Prof. H.-C. Hsueh)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
No. of invited Talks: New FWP

Personnel Commitments for FY2006 to Nearest +/- 10%:

Wei Ku (principle investigator) 10%	Weiguo Yin (postdoc) 0%
S. White (UC Irvine) 10%	Shiu Liu (student) 0%
	Tom Berlijn (student) 0%

Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA 0 K **FY05 BA 0 K** **FY06 BA 410 K**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202030

FWP and possible subtask under FWP:
Condensed Matter Theory
FWP Number: PO-015
Program Scope:
The emphasis of our research program is on strongly correlated electron systems (low-dimensional and frustrated magnets, disordered electrons) and on statistical mechanics of complex systems. Our main topics include:

- Theoretical studies of quantum and classical condensed matter systems, with extension to nano-systems.
- Understanding the evolution, statistical properties and dynamics of complex (particularly biological) systems and their underlying networks.
- Development and application of advanced non-perturbative as well as numerical (first principles) techniques in physics of strongly correlated systems.

Major Program Achievements (over duration of support):

Formulation of a phenomenological theory of the pseudogap state in copper oxide superconductors. Derivation of the universal self energy for d-wave superconductors.

Formulation and testing of the seminumerical method for calculations of spectra and wave functions of coupled of quasi-one-dimensional strongly interacting systems (including quantum dots, coupled chain systems and perturbed integrable systems).

Construction of a systematic technique of quantitatively mapping out the relevant interactions in strongly correlated system, based on first-principles Wannier functions. Development of finite-temperature time-dependent reduced density functional theory. Quantification of electron and lattice interactions for orbital and charge order in manganites. Explanation of gapless CDW in dichalcogenides. Investigation of material dependence of high-Tc cuprates and identification of essential roles of apical oxygen atoms. Development of real space method for the study of local excitons and applied to the explanation of strong anisotropy in NiO and CoO.

The propagation of signals and perturbations in binding networks governed by the law of mass action was studied. The dynamics of SOS network in E. coli was quantitatively modeled. A novel algorithm ranking scientific publications based on underlying citation network was developed and optimized.

The process of charge transfer between a localized electron state and a 1D electron gas was analyzed with an emphasis on the noise generated in this process. Conditions necessary for noise minimization were found. A new low frequency regime of coherent semiclassical dynamics of persistent current qubit was analyzed and a model describing experimental data was developed.

Program impact:
Provided many insights into behavior of strongly correlated systems and properties of complex networks.
Interactions:
Internal: Electron Spectroscopy, X-ray Scattering, Neutron Scattering, Powder Diffraction, CFN, CSC, Biology Dept., Medical Dept.
External: Columbia University (Profs. B. Altshuler and I. Aleiner), ETH Zurich (Prof. T. M. Rice), Harvard University (Prof. E. Demler), MIT (Profs. L. Levitov, T. P. Orlando, Dr. W. D. Oliver), University of Washington, Seattle (Prof. B. Spivak) , University of Wisconsin (Prof. A. Chubukov), Abdus Salam ICTP and SISSA, Trieste, Italy (Prof. V. Kravtsov, Dr. A. Nersesyan, Dr. D. Controzzi), Imperial College, London (Prof. A. Gogolin), Argonne National Laboratory (Dr. V. Vinokur), SUNY at Stony Brook (Prof. A. Abanov), University of Dusseldorf (Prof. R. Egger, Dr. de Martino), Rutgers University (Prof. S. Lukyanov), Niels Bohr Institute, (Prof. K. Sneppen,, S. Krishna), Ariadne Genomics (I. Mazo, Y. Ispolatov, A. Yur'ev, E. Kotelnikova), Univ. of Paris (Prof. B. Roehner), Univ. of Fribourg, Switzerland (Prof. Y.-C. Zhang, M. Blattner), , Tamkang University, Taiwan (Prof. H.-C. Hsueh), University of California, Irvine (Prof. S.R. White), University of Tennessee (A.G. Eguiluz), Boston College (Prof. H. Ding), University of Utah (Prof. D. Mattis), ORNL (B.C. Larson, P. Kent), LANL (C. D. Batista, J. E. Gubernatis)
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
No. of invited Talks: 7 (A. Tsvelik), 5 (S. Maslov), 4 (W. Ku), 4 (R. Konik), 2 (W. Yin)
Personnel Commitments for FY2006 to Nearest +/- 10%:
A.M. Tsvelik (group leader) 100%;Weiguo Yin (postdoc) 100%;S. Maslov 70%;K-K Yan (student) 100%; Wei Ku 90%; Yu. Adamov (postdoc) 100%; R. Konik 100%;D. Voljia (student) 100%; A. Chitov 100%; S. Reyes (student) 100%; D. Walker (student) 100%
Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA 1,410 K **FY05 BA 1,450 K** **FY06 BA 1,450 K**

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP: Biology-inspired programmable assembly of functional nano-structures.
FWP Number: MA-114-MAEA
Program Scope:
The central focus of our research program is to obtain an understanding of the interplay between selective biological interactions and non-selective physical factors for the bio-programmable assembly of hybrid systems. In addition, underlying all work in bio-assembly is the need for a broader library of biological approaches that provide the required selectivity of interaction, and methods for linking the biological elements to the inorganic nano-materials. Our research strategy combines an exploration of the microscopic structure of nanoscale objects with a range of methods for the assembly of such systems, including both biochemical and physiochemical approaches.

Major Program Achievements (over duration of support):
1. Development of methods of synthesis highly mono-disperse nanoparticles (silver, gold, alloy silver-gold) and their functionalization with DNA in a controlled way. Demonstrated that functionalization can be achieved with a controlled total number of DNA as well as a controlled DNA composition.
2. Development of methods for formation of 2D DNA stabilized nanoparticle arrays on silicon surfaces, and studies using AFM, EM and surface x-ray scattering methods. High energy x-ray methods reveal a structure of particle monolayer bound to the surface via hybridized DNA. First studies on kinetic of 2D assembling and temperature reorganization of particle arrays have been conducted.
3. Investigated an effect of DNA composition on assembling. Demonstrated that a kinetic control of DNA driven nanoparticle assembly can be achieved by using DNA conformational changes upon partial hybridization. An enhancement of assembly kinetics by few times was observed, and studied in detail using dynamic light scattering, EM, UV-Vis, and small angle x-ray scattering.
4. Developed methods for tuning interactions between DNA modified particles using various types of DNA. This approach was successfully demonstrated for micron particles, and it was also applied to nanoscale particles. Size of assembly aggregates, kinetics and morphology can be regulated over nearly two orders of magnitude. The systems have been studied using UV-Vis, TEM, dynamic light scattering and small angle x-ray scattering techniques.
5. Study of the interaction between DNA binding proteins, controlling heavy metal resistance in Ralstonia metallidurans, and their specific DNA binding domains. In order to functionalize DNA scaffolds with DNA we selected two DNA binding proteins, PbrR and ArsR, and examined the specificity and the reversibility of their binding to target DNA molecules. This required that we developed the protocols for the expression of soluble, functional forms of these two proteins. Once we obtained sufficient soluble and functional quantities of the two proteins we analyzed their binding to specific DNA fragments by gel retardation studies. Both proteins were found to specifically recognize their own DNA binding sequence. However, we were unable to obtain dissociation of the ArsR protein from its target DNA in the presence of its affector molecule. These two proteins will now be used to functionalize DNA coated particles and DNA scaffolds.
Program impact:
Understanding the assembling of nano-materials in ordered and pre-designed structures will enable a broad array of applications in energy and environmental security.
Interactions:
Internal: BNL-Biology, BNL – MSD/CMP, BNL-Medical
External: University of Michigan, University of Illinois, Stony Brook Univ.
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Platforms for the Integration of Biological Systems into Nanomaterials and Interfaces, Oleg Gang, *Synchrotron Radiation News (2006), to appear in Issue 19.6*

36. A Simple Method for Kinetic Control of DNA-Induced Nanoparticle Assembly
Mathew M. Maye, Dmytro Nykypanchuk, Daniel van der Lelie, and Oleg Gang
JACS Communications (2006), DOI: 10.1021/ja0654229

Personnel Commitments for FY2006 to Nearest +/- 10%:
Oleg Gang (PI) 50%; Daniel van der Lelie (PI): 20%; Dmytro Nykypanchuk (postdoc) 70%; Mathew Maye (postdoc) 70%

Authorized Budget (BA):
FY04 BA - $N/A **FY05 BA -** $360K **FY06 BA -** $345K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP:
Condensed Matter Physics and Materials Science—Soft Matter
FWP Number: PO-034
Program Scope: The primary goal of the group is to understand the effects of nanoscale confinement and the role of self-assembly in soft materials through the use of patterned templates and well-defined interfaces. We use synchrotron x-ray scattering, scanning probe and optical microscopy techniques to study fundamental properties of complex fluids, simple liquids, macromolecular assemblies, liquid crystals, polymers, and biomolecular materials. The challenges are (1) to understand liquids under nano-confinement, (2) how templates and confinement can be used to direct the assembly of biomolecular materials and diblock copolymer thin films, (3) to understand the fundamental interactions which give rise to similar self-assembly behaviour for a wide variety of systems, (4) how the order correlates with function.
Major Program Achievements:

- First verification of shape and size dependent wetting of ethanol on chemically nanopatterned (50-300 nm) lines prepared by oxidation nano-lithography under controlled equilibrium vapor conditions (PRL, 2006). Extended studies, using improved AFM environmental cell, to cyclohexane drops.
- Demonstrated the ability to laterally confine and orient diblock copolymer thin-films by using chemical patterns prepared using oxidation nano-lithography.
- GISAXS observation of ordered 2D arrays of plant virus nanoparticles adsorbed to substrate-supported lipid membranes under buffer solutions. Also probed the effects of lipid charge density and Ca ion.
- Initial FRAP studies of 2D mobility of lipid molecules within substrate supported lipid membranes.
- Lipid monolayer template induced assembly of 2D streptavidin crystallites observed with Brewster-angle microscopy and GISAXS at the solution/vapor interface.
- Initial GISAXS characterization of a well-ordered square array of 20 nm wide cylindrical posts, prepared by e-beam, spaced by 35 nm (100 billion posts). Shows promise as a nanopatterned substrate for wetting studies.
- X-ray scattering study of liquid-supported wetting films to test effects of coupled capillary fluctuations at the two fluid/fluid interfaces and to extract the finite intrinsic interfacial widths (PRE, 2006).
- First direct structural measurements of a thin organic layer, under applied potential, sandwiched between two conductors, by high-energy x-ray reflectivity (PNAS, 2006).
- X-ray photon correlation spectroscopy measurements of the capillary-like dynamics of the free-surface of alkanes in the surface frozen and molten states.
- Microbeam x-ray diffraction study demonstrates that short DNA-oligomers, with minimal shape-anisotropy, still self-assemble into liquid crystalline columnar phases due to end-to-end aggregation.
- Preliminary x-ray studies demonstrated the self-assembly of porphyrin-containing discotic molecules (candidates for photovoltaic applications) into columnar phases.
- The role of tertiary structure in the induction of biominerals was demonstrated in systems containing two-dimensional networks of extracellular matrix protein fibers (PNAS, 2006).

Program Impact: The Groups work has clearly demonstrated the important role that nanopatterned surfaces and templates play in modifying the behavior of liquid, biomolecular materials and polymer films. Studies confirm long-standing theoretical prediction on the effects of the Disjoining pressure on the shape and size of nanodrops. Recognized by an invited talk at the Int. Stat Phys (theory) Conference. The x-ray scattering work at buried liquid interfaces is helping to provide a structural basis for a wide array of interdisciplinary problems ranging from protein crystallization to molecular electronics. The work on Electro Pen Nanolithography provides a new means of preparing chemically patterned surfaces (patent application pending).
Interactions: This is a joint project among researchers in three BNL departments: Condensed Matter Physics and Materials Science, the National Synchrotron Light Source, and the Center for Functional Nanomaterials.
Recognitions, Honors and Awards (at least partly attributable to support under this FWP/subtask):
Invited Talks 8, Antonio Checco received the Pierre Favard 2005 award for the best PhD thesis in Microscopy between 2002-2005. This award is given by the French Society of Microscopy. Brookhaven Science and Technology Award – B. Ocko. 2 earlier APS fellows.
Personnel Commitments for FY2006: Ben Ocko (0%), Brandon Chapman (100%), Elaine DiMasi (10%), Ron Pindak (10%), Lin Yang (10%), Antonio Checco (100%), Masa Fukuto (100%), Julian Baumert (50%), Suntao Wang (100%)
Authorized Budget (BA): F**Y04 BA** - $742K **FY05 BA** - $690K **FY06BA** - $630K